187

# JOURNAL OF MOLECULAR SPECTROSCOPY

LIBRARY USE ONLY
UNIVERSITY OF HAWAII
LIBRARY

VOLUME 33, 1969

*Editors*

Harald H. Nielsen K. Narahari Rao

*Editorial Advisory Board*

G. Amat
Børge Bak
H. J. Bernstein
J. Brandmüller
Bryce L. Crawford, Jr.
David M. Dennison
Hs. H. Günthard
H. S. Gutowsky
G. Herzberg
Jon T. Hougen
K. K. Innes
Richard C. Lord
P.-O. Löwdin
Ross A. McFarlane
A. Mangini
M. Migeotte
Ian Mills
Yonezo Morino
Robert S. Mulliken
John G. Phillips
J. Plíva
G. Wilse Robinson
H. L. Welsh
E. Bright Wilson, Jr.

ACADEMIC PRESS

NEW YORK and LONDON

Copyright © 1970, by Academic Press, Inc.

ALL RIGHTS RESERVED

No part of this volume may be reproduced in any form by photostat, microfilm, by retrieval system, or any other means, without written permission from the publishers.

*Made in the United States of America*

# CONTENTS OF VOLUME 33

Number 1, January 1970

Ronald G. Selsby and R. C. Nelson. The Ionization Energy of Cationic Cyanine Dyes 1

M. Witanowski and S. A. Shevelev. Nitrogen-14 Nuclear Magnetic Resonance and Molecular Orbitals in Nitrocarbanion Systems 19

B. H. Schechtman and W. E. Spicer. Near Infrared to Vacuum Ultraviolet Absorption Spectra and the Optical Constants of Phthalocyanine and Porphyrin Films 28

Jimmie R. McDonald, James H. Wharton, and Robert V. Nauman. Absorption and Emission Spectra of 2,3-Benzobiphenylene—Comparison with Pariser-Parr-Pople SCF-MO-CI Calculations 49

Ira W. Levin. Potential Function for Phosphorus Pentafluoride 61

E. G. Finer, R. K. Harris, M. R. Bond, R. Keat, and R. A. Shaw. Proton Spectra of Symmetrical Cyclotriphosphazatrienes 72

A. Warshel, M. Levitt, and S. Lifson. Consistent Force Field for Calculation of Vibrational Spectra and Conformations of Some Amides and Lactam Rings 84

G. Sbrana and V. Schettino. Vibrational Spectra and Isomerism in Propyl- and Butylaldehydes 100

R. E. Blank, M. D. Olman, and C. D. Hause. Upper State Molecular Constants for the (0, 0, 3) and (1, 0, 3) Vibration-Rotation Bands of Nitrogen Dioxide 109

K. K. Yee, W. E. Jones, and I. Kopp. Emission Spectrum of the PSb Molecule 119

R. M. Lees. Linear Dependence in Least Squares Analysis, with an Application to Internal Rotation 124

C. M. Pathak and H. B. Palmer. New Electronic Transitions in TiO 137

G. Herzberg. The Dissociation Energy of the Hydrogen Molecule 147

NOTES

Bhanu Pratap Singh. Orbital Valence Force Field in Halogenated Ions of IIIA Group 169

Richard H. Cox. Substituent Effects on Long-Range Proton-Fluorine Coupling Constants: Substituted Benzotrifluorides 172

Anthony Ficarra, Suei-Rong Huang, and Anthony A. Reid-

LINGER. Intramolecular Screening Effects on Proton Chemical Shifts in 1,8-Diaminoperchloronaphthalene 175
Y. MIKAWA AND R. J. JAKOBSEN. Lattice Vibrations of Crystalline Formic Acid 178
G. C. ALLEN AND KEITH D. WARREN. Vibrational Fine Structure in the $^1A_{1g} \rightarrow {}^1T_{1g}$ Band of the Hexafluoronickelate (IV) Anion 180

LETTER TO THE EDITOR

W. R. L. CLEMENTS AND B. P. STOICHEFF. High-Resolution Raman Spectroscopy of Gases with Laser Excitation 183

Papers Accepted for Publication 187

NUMBER 2, FEBRUARY 1970

V. SETHURAMAN, V. A. JOB, AND K. K. INNES. The 3500 Å $^1A_2 - {}^1A_1$ Transition of Formaldehyde-$h_2\,d_2$ and $h\,d$. Analysis of Coriolis and Fermi Perturbations 189
G. R. BIRD, G. R. HUNT, H. A. GEBBIE, AND N. W. B. STONE. The Far-Infrared Pure Rotational Spectrum of Nitrogen Dioxide ($NO_2$) 243
M. B. ROBIN AND N. A. KUEBLER. Pressure Effects on Vacuum Ultraviolet Spectra 274
LAWRENCE EDWARDS AND MARTIN GOUTERMAN. Porphyrins. XV. Vapor Absorption Spectra and Stability: Phthalocyanines 292
C. M. WOODMAN. The Absorption Spectrum of HNF in the Region 3800–5000 Å 311
WALTER J. LAFFERTY, ARTHUR G. MAKI, AND THOMAS D. COYLE. High Resolution Infrared Spectrum and Structure of Diborane 345
V. ŠPIRKO AND J. MORÁVEK. Solution of the Inverse Secular Problem by "Monte Carlo" Method 368

NOTES

LLEWELLYN H. JONES. Comment on paper, "Some Properties of the Eigenvector Matrix in the Theory of Molecular Vibrations" 375
G. W. KING AND S. P. SO. Allowed and Forbidden Components in the 2790 Å System of Ethynylbenzene 376
Papers Accepted for Publication 379

NUMBER 3, MARCH 1970

M. A. A. CLYNE AND J. A. COXON. The Visibile Band Absorption Spectrum of Chlorine 381
MASAO SUZUKI AND KUNIO KOZIMA. Microwave Spectra, Barrier Heights to Internal Rotation of Methyl Group and Dipole Moments for Conjugated Chain Compounds: *trans*-Crotononitrile 407
J. R. DICKINSON AND K. E. JOHNSON. Electronic Spectrum of Cobalt (II) in Sulfates. Sulfuric Acid Solutions 414

Daniel Højgaard Christensen and Ole Faurskov Nielsen. Potential Function of Dichlorosilane 425
H. F. Shurvell and J. A. Faniran. The Infrared and Raman Spectra of Solid Trifluoroacetonitrile 436
David R. Lide, Jr. Determination of Anharmonic Potential Constants in Linear $XYZ$ Molecules 448
Eizi Hirota and Yonezo Morino. Microwave Spectrum of Phosphorus Trifluoride. Molecular Structure and Force Constants 460
H. J. Jakobsen and J. AA. Nielsen. Nuclear Magnetic Resonance of Organophosphorus Compounds. $^{1}H$-$^{31}P$ Spin Coupling Constants in Some Heteroaromatic Phosphines and their Derivatives 474
M. S. Child. Repulsive Potential Curves from Predissociation Data 487
J. B. Moffat and C. Vogt. The Electronic Structure and Nonplanarity of Cyanamide 494
Josef Plíva. The Photographic Infrared Bands $5v_3$ and $4v_2^0 + 4v_3$ of $^{14}N_2{}^{16}O$ 500
S. G. Tilford, M. L. Ginter, and Joseph T. Vanderslice. Electronic Spectra and Structure of the Hydrogen Halides. The $b^3\Pi_i$ and $C^1\Pi$ States of HCl and DCl 505
Ch. Jungen and H. Lefebvre-Brion. The Quandrupole Moment of $NO^+$ 520
Robert J. Capwell, Jr., and Gerd M. Rosenblatt. Infrared Spectrum of Condensed $As_4$ and Thermodynamic Functions of $As_4$ Gas 525
R. Yamdagni. Absorption Spectrum of SnSE Molecule in the Visible Region 531
Takehiko Tanaka and Yonezo Morino. Coriolis Interaction and Anharmonic Potential Function of Ozone from the Microwave Spectra in the Excited Vibrational States 538

NOTES

Takehiko Tanaka and Yonezo Morino. Band Origin of the $v_2$ Fundamental of Ozone 552
C. N. R. Rao, G. C. Chaturvedi, and S. N. Bhat. Vapor Phase Charge-Transfer Spectra of Iodine Complexes 554
A. Ruoff and W. Sawodny. The Force Field of Methinophosphide 556

ANNOUNCEMENT 559

Papers Accepted for Publication 561
Author Index 562
Subject Index 564